Combining ensemble and variational data assimilation

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Award Number: N62909-10-1-7068
including partial support from ONR Global's Naval International
Cooperative Opportunities Program (NICOP)
http://www.cmar.csiro.au/staff/oke/onr.htm
http://ingria.coas.oregonstate.edu

LONG-TERM GOALS

The long-term goal of this project is to develop and apply practical methods for data assimilation to improve the short-range prediction of mesoscale ocean variability.

OBJECTIVES

A key objective of this work is to develop an ocean data assimilation system that exploits the strengths of both the ensemble-based (e.g., Evensen 2003; Houtekamer and Mitchell 1998; Tippett et al. 2003) and variational (e.g., Bennett 2002) approaches to data assimilation. The first step in this project is to perform an inter-comparison of an ensemble-based data assimilation system with a 4dVar system for a suite of coastal model configurations. The second step is to identify the strengths and weaknesses of each system and to improve both systems by *borrowing* components from the other system. It is our goal to develop a hybrid ensemble-var system. We will investigate the extent to which the ensemble-var system can outperform both the ensemble-based and variational approaches, both in terms of forecast skill (accuracy) and computational efficiency (throughput).

APPROACH

An ensemble-based data assimilation system, based on an Ensemble Optimal Interpolation (EnOI) scheme (Oke et al. 2002; Evensen 2003), has been developed and tested for a range of applications by Dr. Oke (Oke et al. 2005; 2008; 2009; 2010; 2013a), and a 4dVar system, based

Report Documentation Page

Form Approved
OMB No. 0704-0188

1. REPORT DATE **30 SEP 2013**	2. REPORT TYPE	3. DATES COVERED **00-00-2013 to 00-00-2013**
4. TITLE AND SUBTITLE **Combining ensemble and variational data assimilation**		5a. CONTRACT NUMBER 5b. GRANT NUMBER 5c. PROGRAM ELEMENT NUMBER
6. AUTHOR(S)		5d. PROJECT NUMBER 5e. TASK NUMBER 5f. WORK UNIT NUMBER
7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES) **Oregon State University,College of Oceanic and Atmospheric Sciences,104 COAS Administration Building,Corvallis,OR,97331-5503**		8. PERFORMING ORGANIZATION REPORT NUMBER
9. SPONSORING/MONITORING AGENCY NAME(S) AND ADDRESS(ES)		10. SPONSOR/MONITOR'S ACRONYM(S) 11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION/AVAILABILITY STATEMENT
Approved for public release; distribution unlimited

13. SUPPLEMENTARY NOTES

14. ABSTRACT

15. SUBJECT TERMS

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT **unclassified**	b. ABSTRACT **unclassified**	c. THIS PAGE **unclassified**	**Same as Report (SAR)**	**16**	

Standard Form 298 (Rev. 8-98)
Prescribed by ANSI Std Z39-18

on the representer method (Chua and Bennett 2001; Bennett 2002), has been developed and tested for coastal ocean applications by Dr. Kurapov (Kurapov et al. 2007, 2009, 2011, Yu et al., 2012).

Conceptually, both the ensemble and variational approaches perform analogous tasks. Both implicitly generate estimates of the system's background error covariance, both interpolate and extrapolate background innovations (model-observation differences) onto the full model state (including all variables at all model grid points), and both seek to minimize some norm of the model-observation misfits. The ensemble-approach has an advantage that it uses the Non-Linear Model (NLM) operator to generate and evolve the system's error covariance, but has the disadvantage that it is rank deficient (i.e., uses too few ensemble members to completely span the error sub-space of the system). The variational representer-based approach, by contrast, is full rank, but it uses linear operators (Tangent Linear Model, TLM; and Adjoint Model, ADM) to derive the system's error covariance, or representers. The ensemble-approach is typically implemented as a three-dimensional interpolation (e.g., Oke et al. 2005; 2008; 2013a) – though four-dimensional filters have been tested for intermediate models (e.g., Sakov et al. 2010) and the representer-approach is fundamentally four-dimensional (Kurapov et al. 2007, 2009; 2011). There are pros and cons of both approaches. Under this project, we are seeking to exploit the strengths of both approaches, with the goal of developing a superior ensemble-var data assimilation system.

In this project we apply an EnOI and 4dVar assimilation system to the same application. This has been achieved with the application of the Advanced Variational Regional Ocean Representer Analyzer (AVRORA; Kurapov 2009), a 4dVar system, to the Bonney Coast, off Southern Australia – the region of strongest wind-driven upwelling off Australia's shores. This application has facilitated two important analyses. Firstly, this has permitted a demonstration that a ROMS-based TLM and ADM can be successfully used to initialise a different NLM. Secondly, this has permitted a direct comparison of ensemble-based and 4dVar-based representers and analyses – using the same NLM, with the same surface forcing, topography, boundary forcing, and so on. Specifically, we have tested the assumption that a 4dVar-based assimilation requires the specific "companion" TLM and ADM, by applying a ROMS-based TLM and ADM to a different, independent NLM – the Sparse Hydrodynamic Ocean Code (SHOC; Herzfeld 2009). Our results show that indeed, the ROMS-based TLM and ADM can be used to successfully initialize a SHOC.

Dr. Peter Oke and Dr. Alexandre Kurapov are the P.I.s on this project and lead the ocean data assimilation activities at CSIRO Marine and Atmospheric Research and Oregon State University (OSU), respectively. Dr. Oke and Dr. Kurapov are working closely together under this project, in collaboration with Dr. Chaojiao Sun, Dr. Emlyn Jones, and Dr. Terrence O'Kane from CSIRO, and Dr. Sangil Kim, formerly from OSU. To facilitate this collaboration, Dr. Kurapov visited CSIRO between 8-12 October 2012, and Dr. Sun visited OSU between 7-18 January 2013. Beginning Fall 2013, a new student - Mr. Ivo Pasmans - will join the OSU team to contribute to the success of this project on combined ensemble-variational assimilation in coastal ocean circulation modeling; and a new student – Mr. Hugo Bastos de Oliveira – will join the CSIRO team to contribute to the success of this project in coastal ocean data assimilation.

WORK COMPLETED

A series of assimilation experiments using the ensemble-based data assimilation system developed by Dr. Oke has been completed using SHOC for the Bonney coast, for south-east Tasmania, and

for a region around the Hawaiian Islands. These regions span different dynamical regimes, testing the assimilation system across a range of different scenarios. Results from the experiments off the Bonney coast are being prepared for publication, results from the experiments off south-east Tasmania have been published (Jones et al. 2012), and results from the experiments around Hawaii have been published (Oke et al. 2013b).

The ROMS-based 4dVar system developed by Dr. Kurapov has been applied to the Bonney coast. The ROMS-based 4dVar system has been applied to configurations of both ROMS and SHOC for the Bonney Coast. The application to SHOC is the first known demonstration that a TLM and ADM from one NLM can be used to successfully initialise a different NLM. Results from these experiments are being prepared for publication.

A series of comparisons between 4dVar-derived representers, and ensemble-based representers has been completed, highlighting the strengths and weaknesses of the different techniques. Analysis of the ensemble-based representers has been used to underpin an initial evaluation of the "footprint" (the region that is well-monitored) of the Australian Integrated Marine Observing System (IMOS; www.imos.org.au). Results from this analysis have been published (Oke and Sakov, 2012).

In addition to the efforts along the Bonney coast, we continued testing and improving the OSU AVRORA assimilation system. Some tests were applied to coastal ocean flows off Oregon, where dynamics are well studied (Oke et al., 2002, Kurapov et al., 2003, 2005, Springer et al., 2009, Koch et al., 2010, Osborne et al., 2011). In particular, the study of the impact of assimilation of high-frequency (HF) radar surface currents has been completed (Yu et al., 2012). In terms of further model and assimilation system improvement, our focus was on adding the Columbia River discharge, to study how assimilation of surface and hydrographic section data can be done optimally in the presence of a large river plume. To be able to model the Columbia River dynamics, we extended the model domain to include both Oregon and Washington coasts. Tidal forcing has been added to help mixing river and ocean waters in the estuary. The resolution has been improved to 2-km in horizontal. The heat flux component of ROMS has been modified to allow variable shortwave attenuation (smaller attenuation depth in the area of the river plume, simulating the effect of more turbid waters within the plume). Analysis of adjoint sensitivity fields and representer functions has been done, comparing zones of influence of the data in cases with and without the river plume. As discussed below, results suggested that combining ensemble and variational data assimilation may be particularly beneficial when assimilation of the surface data is performed in the presence of the anomalously thin and stratified surface layer associated with the river plume.

RESULTS

Experiments applying an ensemble data assimilation system, based on EnOI (Oke et al. 2002), have been performed for the Bonney coast during a series of wind-driven upwelling events; for a region off south-east Tasmania during a series of glider deployments; and around the Hawaiian Islands, for an open-ocean tropical case (Oke et al. 2013b). In parallel, experiment applying the 4dVar system, using AVRORA (Kurapov 2009), have been performed for the Oregon coast. A series of ensemble- and 4dVar-based representer functions have been compared, providing

insights into the impact of different observations on a data-assimilating model for a range of different scenarios (e.g., upwelling, river plume event).

Hawaiian Islands ensemble-based study

For this study, we use the latest version of BODAS – that is used here is described by Oke et al. (2013a). We assimilate sea-level anomaly (SLA) from satellite altimetry, satellite sea-surface temperature (SST), and in situ profiles of temperature and salinity from Argo floats (*Figure 1*). We intentionally with-hold temperature profiles from XBT surveys to use for independent evaluation. We find that the resulting modeled SLA and SST fields are in excellent agreement with assimilated observations. For example, the mean and standard deviation of SST from verifying analyses (i.e., gridded observations) and the model are shown in *Figure 2*. These comparisons confirm that the model is well constrained to observations – with both the mean circulation and the modeled variability closely matching the observations.

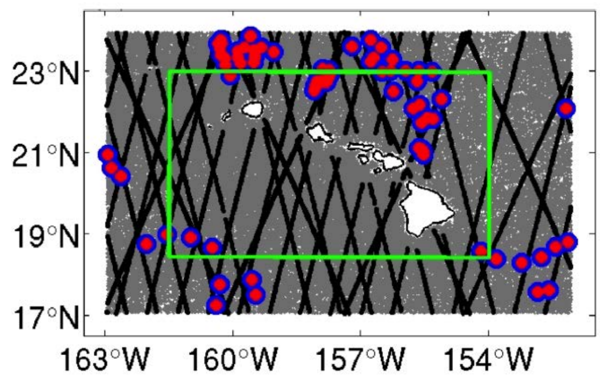

Figure 1: The Map showing the extent of the model domain (green) and the location of assimilated observations of SST (grey), atSLA (black), temperature (blue) and salinity (red) profiles. The locations of all assimilated observations used in each 60-day period are shown. The coverage of the SST observations denotes the domain for which analyses are computed during the assimilation step.

[Figure shows that the are many assimilated temperature and salinity profiles to the north of the Hawaiian Islands, but very few to the south and west.]

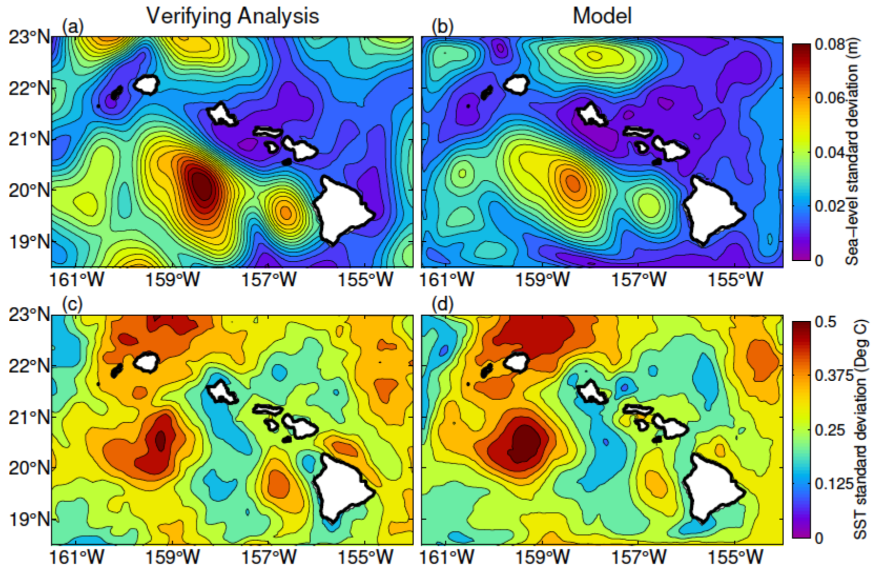

Figure 2: Comparison of the standard deviation of (a-b) sea-level and (c-d) SST from (a,c) the verifying analysis and (b,d) the model for the case study being presented.
[Figure shows the good agreement between the observed and reanalysed SST.]

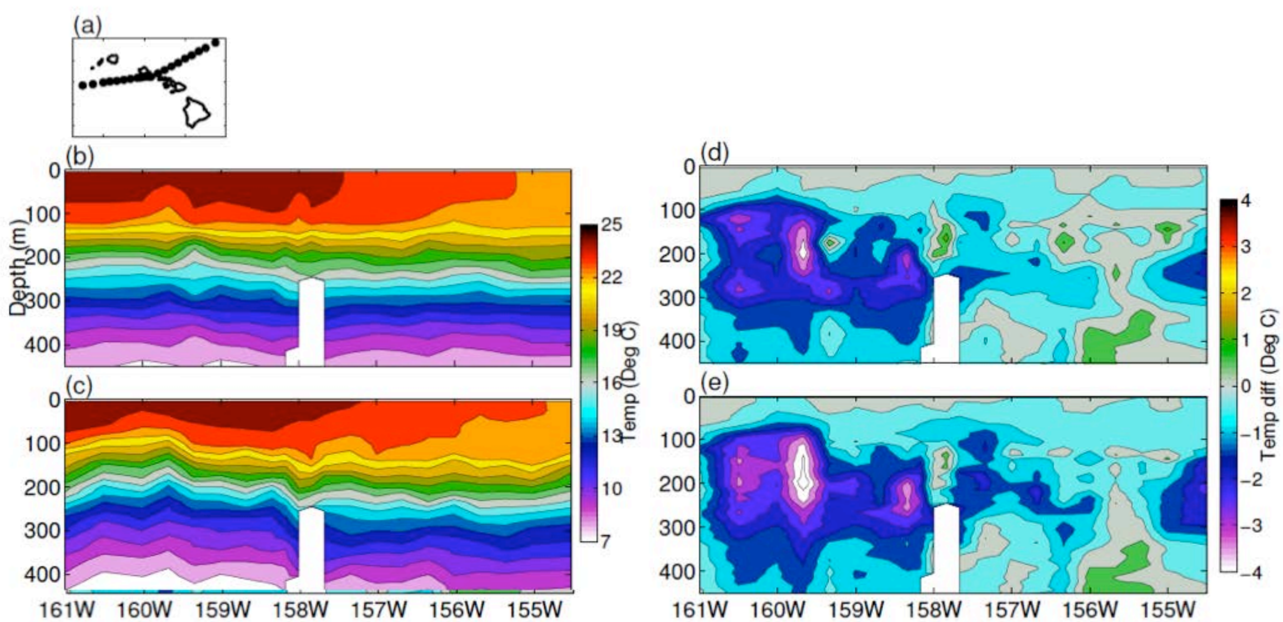

Figure 3: Temperature section along (a) an XBT transect (PX-34) showing the (b) observed and (c) modelled temperature over the top 450 m; and the difference between the observed temperature and the (d) modelled and (e) analysed temperature. The XBT section spanned 16-18 February 2008.
[Figure shows that the reanalyzed subsurface temperature closely matches independent observations to the north and east of the Hawaiian Islands, where there are plenty of assimilated observations]

South-east Tasmanian study

The study off south-eastern Tasmania (Jones et al. 2012) used the SHOC model nested inside the Bluelink ReANalysis (BRAN; Oke et al. 2013a) to investigate the degree to which in situ observations from a sparse array of moorings and from gliders can constrain a high-resolution coastal ocean model; and to investigated the ability of an EnOI-based system to constrain a model that has a significant temperature bias. In areas with dense observations, the assimilation scheme reduced the root-mean-squared (RMS) difference between the model and independent with-held satellite sea-surface temperature (SST) observations by 90%, while the domain-wide RMS differences were reduced by a more modest 40%. Their findings showed that errors introduced by surface and boundary forcing can be identified and reduced by a relatively sparse observing array using an inexpensive ensemble-based data assimilation system.

Bonney coast ensemble-based study

The study off the Bonney coast used a 2-km resolution configuration of the SHOC model and includes a suite of different configurations where SHOC is nested inside a different "parent models", including: BRAN - large-scale 1/10^{o}-resolution ocean reanalysis (BRAN; Oke et al. 2013a); BRAN plus observations – where the BRAN fields are combined with high-resolution observations of SLA, SST, and in situ temperature and salinity (retaining more observations than the original BRAN run, and performing an assimilation more frequently in time); and climatology plus observations – where a seasonal climatology is combined with observations of sea-level anomaly, sea-surface temperature, and in situ temperature and salinity. This study showed that good agreement with observations is achieved for each configuration – even the case initialised with only climatology and local observations.

4dVar-based Oregon study

In AVRORA tests off Oregon, we found that assimilation of HF radar surface currents helps improve not only velocity forecasts, but also estimates of SST fronts. In particular, as a result of assimilation of currents, the model-data SST correlation is improved (Yu et al., 2012). These results encouraged us to approach analysis and assimilation of the HF radar observations off the Bonney Coast.

As a pre-requisite to data assimilation, dynamical analyses of the model cases with and without the Columbia River have been performed. The results are described in (Kurapov et al., 2013). These analyses demonstrated that SST is relatively warmer in the area of the plume. This effect is stronger in the case with the variable shortwave radiation attenuation depth (where the attenuation depth is smaller in the area of the plume). At the same time SST inshore of the river plume (which was turned to south of the river mouth due to upwelling favorable winds) is relatively colder, as an effect of changes in the surface boundary layer (*Figure 4*).

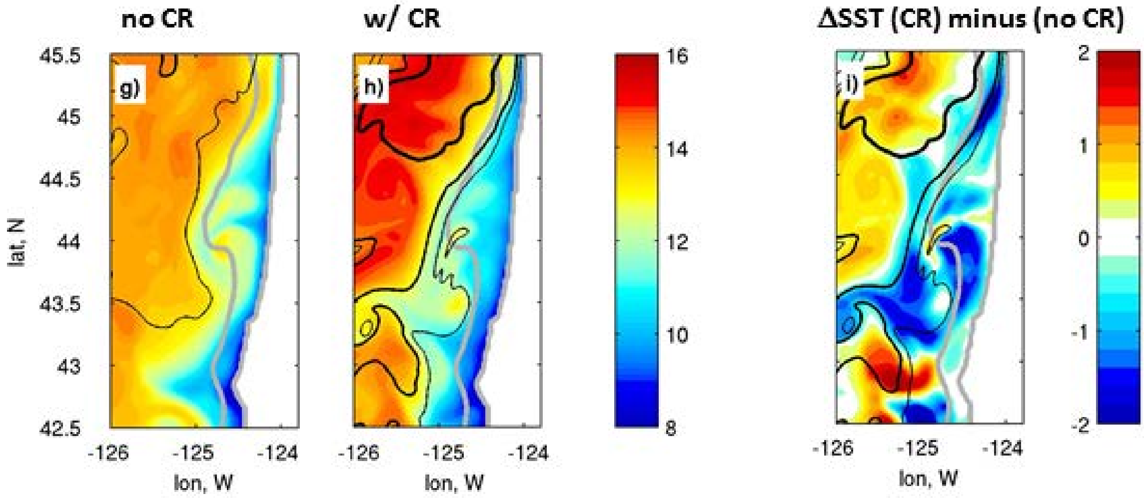

Figure 4: Model daily average SST (color) and SSS (contours, 30, 32, and 32.5 psu): (left to right) model w/ no Columbia River (CR), model w/ CR, difference between the two cases. SST in the area of the river plume is warmer than in the case w/out CR. SST inshore of the river plume is colder. Assimilation in the presence of the river plume requires a dynamic initial condition error covariance that may be computed using ensemble methods.
[Figure shows the far-reaching impact of the Columbia River]

Analysis of adjoint sensitivities (outputs of the ADM) corresponding to observations of the surface velocity and SST has shown that the river plume strongly affects areas of impact of these observations in a data assimilation system. Since the adjoint sensitivity fields may be interpreted as model error covariances between the observed variable and model initial fields given the assumption of uncorrelated initial errors, our finding suggests that strongly non-homogenous covariances must be assumed for the initial conditions in the 4DVAR cost function in the area of the river plume. Such a covariance might be most conveniently built using an ensemble of forecasts, which will account for non-homogeneity associated with the presence of the river plume.

To make steps in this direction, we are currently building and analyzing covariances based on ensembles of ROMS solutions. These are obtained by perturbing the forcing wind velocity fields along directions provided by the Empirical Orthogonal Functions (*Figure 5*). After software for obtaining these covariances is fully tested, we will run tests comparing data assimilation results with the ensemble-based and more traditional (Gaussian, dynamically based – see Weaver et al., 2005, Kurapov et al., 2011, Yu et al., 2012) covariance.

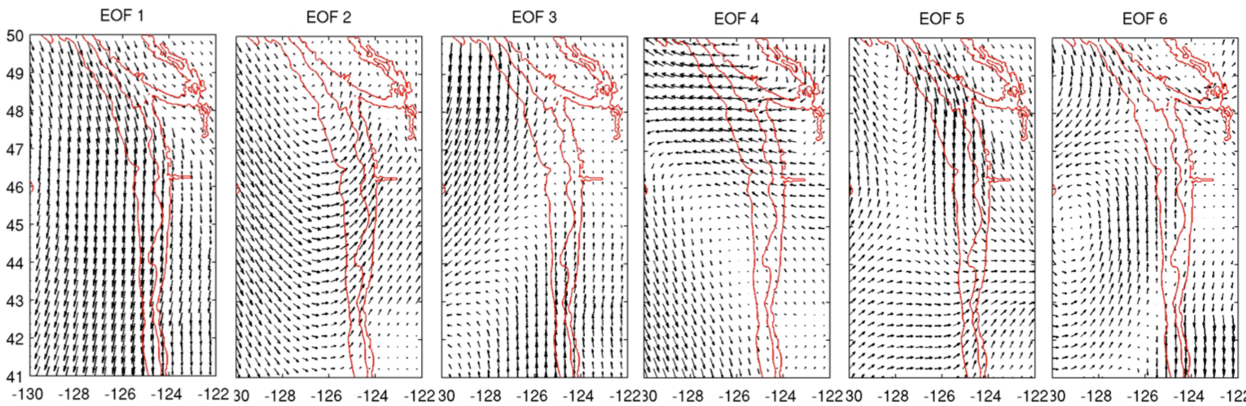

Figure 5: The ensemble of model solutions to form the ensemble-based covariance for 4DVAR will be built using the dominant modes of variability of the wind forcing (so called Empirical Orthogonal Functions). The 6 most important EOFs are shown in this figure, corresponding to upwelling conditions. Contours are the coast and 200 and 2000 m isobaths.

Application of ROMS-based 4dVar to SHOC off the Bonney coast

An example of results from an experiment where the ROMS-based 4dVar system (Kurapov et al. 2009) is applied to SHOC is presented in *Figure 6*. This example is during a strong upwelling-favourable wind event. The prior model solution (*Figure 6b*, derived from SHOC) shows only a weak signature of the upwelling, with moderately cold water adjacent to the coast. By contrast, the posterior analysis (*Figure 6*c, derived using the ROMS-based 4dVar tools and using the SHOC prior solution) shows a much stronger signature of upwelling adjacent to the coast, with a plume of cold upwelled water extending to the east at about 37°S, in good agreement with the assimilated observations (*Figure 6*a). For this example, the 4dVar-derived increment to SST shows an intensification of the cold upwelling signature near the coast and a temperature increase offshore that is “correcting” an unobserved filament of cold water (*Figure 6*d). For these experiments, we configure SHOC and ROMS with the same horizontal grid, using the same topography, using the same surface forcing, and the same horizontal boundary forcing. However, ROMS uses a terrain-following vertical coordinate (s-coordinate) and SHOC uses a z-level vertical coordinate. The SHOC prior solution is prepared for the assimilation by interpolating the SHOC fields onto the ROMS grid.

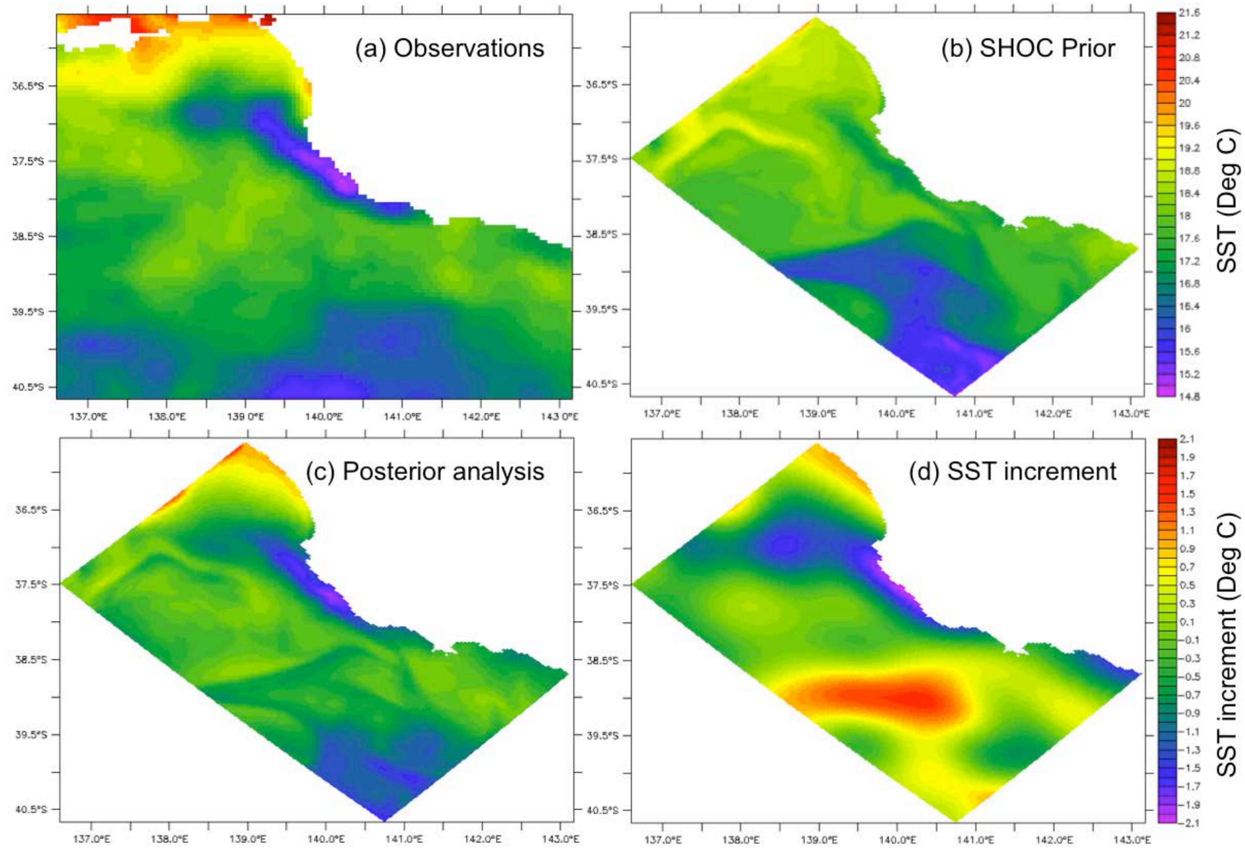

Figure 6: Example of SST on 1 February 2012 from (a) observations, (b) SHOC prior solution, (c) SHOC posterior analysis, and (d) 4dVar-derived SST increments during an upwelling event off the Bonney coast, off Southern Australia.
[Figure showing the successful application of a ROMS-based 4dVar system to a different ocean model (SHOC).]

Comparison of ensemble- and 4dVar-based representers

An example of an ensemble- and 4dVar-derived normalized representer function for an SST observation in the upwelling region off the Bonney coast is presented in *Figure 7*. In this example, the "footprint" – or region of influence – of the observation shows a similar anisotropic structure in both estimates of the representer. Note that the ensemble-based representer is derived from a time-invariant 180-member ensemble of intraseasonal model anomalies, following the approach used by Oke et al. (2013a). By contrast, the 4dVar-based representer is derived using the ROMS-based TLM and ADM, and is dependent on the prior solution – that is here taken from the SHOC model during the upwelling event depicted in *Figure 6*. The region of influence of the SST observation is clearly smaller in the 4dVar-based representer function (*Figure 7*). The region of the typical upwelling plume is clearly evident in the ensemble-based representer, extending the extent of the region model domain.

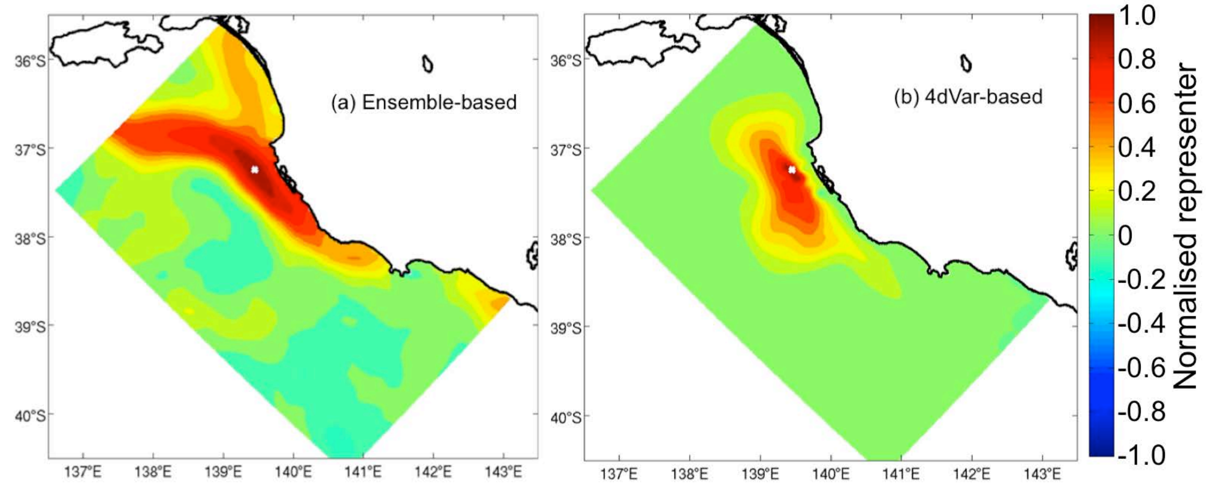

Figure 7: Examples of an ensemble- and 4dVar-based normalised representer function for a temperature observation in the upwelling zone off the Bonney coast. The cross in each panel denotes the location of the observation.
[Figure comparing an ensemble- and 4dVar-derived representer function.]

Exploitation of representer functions

We define the "footprint" of an ocean observation as the region that is well correlated to the observed variable at zero time-lag. The footprint of observations from an observation array provides an indication of the region that is effectively monitored by that array. Oke and Sakov (2012) examine the footprint of moorings that underpin the Australian IMOS (www.imos.org.au). Based on sea-surface height, temperature, and velocity from a 17-year model run, we quantify the footprint of existing moorings to identify the extent to which the shelf circulation is likely to be represented by those moorings. We find that in combination, the nine long-term National Reference Stations (NRSs) effectively monitor, with a correlation of >0.8, the interannual (intraseasonal) variability of the shelf circulation in about 80% (30%) of the region around Australia. The 28 additional IMOS moorings expand the combined footprint for intraseasonal variability to cover up to 70%. We identify several gaps in the IMOS that could be filled by additional observations, including the regions off the east coast, the central Great Barrier Reef, the Great Australian Bight, parts of the north–west shelf, and the Gulf of Carpentaria. The assessment of IMOS performed by Oke and Sakov (2013) is preliminary – limited to hypothetical observations of surface height, surface temperature, and surface velocity. A more comprehensive assessment of IMOS is planned.

IMPACT/APPLICATIONS

Most applications of ensemble data assimilation assume that a model and assimilated observations are unbiased. However, it is common for both models and observations to have some degree of bias. Models particularly, often develop a bias due to errors in either surface or boundary forcing. The study by Jones et al. (2012) demonstrated that a simple EnOI-based system can be used to identify model bias, and to correct the bias, even with a relatively sparse set of observations. This means that the commonly adopted assumption by data assimilation systems that a model is

unbiased – is not necessarily a fatal flaw of a data-assimilating model. The study described by Jones et al. (2012) also demonstrated that a sparse array of in situ observations, from moorings and gliders – with no assimilation of satellite observations – can successfully constrain a high-resolution coastal ocean model.

The finding that a high-resolution coastal ocean model that is nested within climatological fields combined with observations yields a solution that is in close agreement with observations is important. For operational purposes, such a system could be run independently of a large-scale "parent" system that is often a global-scale eddy-resolving ocean forecast system. Such global systems typically require massive super-computing resources. By contrast, a relatively small coastal model can be run on a much smaller computing platform – perhaps from a remote facility with minimal access to main-stream computational resources. In such a case, the coastal model requires only access to two-dimensional atmospheric forcing fields and observations for the region of interest.

The demonstration that a TLM and ADM from one model can be successfully applied to a different model, may open the door for the development of a suite of community 4dVar data assimilation tools. To date, the application of 4dVar to a given model has been assumed to require the development and maintenance of a *companion* TLM and ADM. Under this project, we've shown that a ROMS-based TLM and ADM can be successfully applied to the SHOC model. The robustness of this capability needs to be tested – for example through the application of a ROMS-based (or other) TLM and ADM to a range of different community models (e.g., POM, HYCOM, NCOM, NEMO etc.).

Since the adjoint sensitivity fields may be interpreted as model error covariances between the observed variable and model initial fields given the assumption of uncorrelated initial errors, our finding suggests that strongly non-homogenous covariances must be assumed for the initial conditions in the 4DVAR cost function in the area of the river plume. Such a covariance might be most conveniently built using an ensemble of forecasts, which will account for non-homogeneity associated with the presence of the river plume. This provides an additional motivation to combining ensemble and variational methods.

Representer functions, derived either from a 4dVar system or an ensemble data assimilation system contain important information for the design and assessment of observing systems. The study of Oke and Sakov (2012) provided a preliminary assessment of the Australian IMOS. A similar study should be extended to include the impact of other observations, including sub-surface observations from moorings, gliders, and profiling floats, and other satellite observations. Moreover, the approach of Oke and Sakov (2012) could also readily be applied to other regions to evaluate the effective coverage of other long-term monitoring platforms (e.g., TAO array, other national and international observing systems.

RELATED PROJECTS

Enhancing the Pacific Northwest Regional Coastal Observing System (RCOOS) of NANOOS, NOAA, PI (2008-2013); *Ocean Surface Currents from SST: Derived Motion and Model Data Assimilation*, NOAA-GOES-R (via CIOSS) PI, 10/1/2012-09/30/2013; *GOES SST Assimilation for Nowcasts and Forecasts of Coastal Ocean Conditions*, NOAA-GIMPAP (via CIOSS),10/1/2012-

09/30/2013, PI: Using leverage by these projects, we designed and supported the Oregon real-time coastal ocean forecast system. It uses the AVRORA 4DVAR assimilation component to assimilate alongtrack altimetry (Jason-1, Jason-2, CryoSat), hourly SST from GOES, and surface currents from an array of HF radars. The system provides every-day updates of 3-day forecasts of ocean currents, SST, and other variables of interest. These have been provided to NOAA via an OpenDAP server. NOAA utilized our fields to track marine debris objects (including large objects, like docks, floating toward the US West Coast from Japan, released into the ocean during the 2011 Tsunami). In these projects we have learned about the impact of SST and altimetry on the quality of the forecasts (Kurapov et al., 2011, Yu et al., 2012).

MURI: Remote Sensing and Data Assimilative Modeling in the Littorals, ONR, 2010-2015, co-PI (w/ A. Jessup (lead), S. Edgar, R. Holman, M. Haller, T. Ozkan-Haller et al.): In this project, we have developed the adjoint counterpart of a coupled wave-circulation model and studied the impact of velocity observations on bathymetry correction in the nearshore surf zone (Kurapov and Ozkan-Haller, 2013). This study allowed us understanding some common issues with regard to assimilation in coupled models.

Bluelink is a partnership between CSIRO, the Bureau of Meteorology and the Royal Australian Navy (http://wp.csiro.au/bluelink/). Many of the research activities undertaken in Bluelink have strong synergies with the project that is the subject of this annual report. The main objective of Bluelink is the development and application of an ocean forecast system for the mesoscale circulation around Australia. Applications of the Bluelink system are well documented (e.g., Oke et al. 2005; 2008; 2009; 2010; Schiller et al. 2008). Results from version 3 of the BRAN – BRAN3 are described by Oke et al. (2013a). In this study, Oke et al. (2013a) present results from a second-generation eddy-resolving ocean reanalysis that is shown to match both assimilated and with-held observations more closely than its predecessor; but involves much smaller adjustments to the model state at each assimilation. They compare results from BRAN2 (Schiller et al. 2008) and BRAN3 (Oke et al. 2013a) in the Australian region. Overall, the misfits between the model fields in BRAN3 and observations are 5-28% smaller than the misfits for BRAN2. Specifically, they show that for BRAN3 (BRAN2p5) the sea-level, upper ocean temperature, upper-ocean salinity, and near-surface velocity match observations to within 7.7 cm (9.7 cm), 0.68^{o}C (0.95^{o}C), 0.16 psu (0.18 psu), and 20.2 cm/s (21.3 cm/s) respectively. Oke et al. (2013a) also show that the increments applied to BRAN3 - the artificial adjustments applied at each assimilation step - are typically 20-50% smaller than the equivalent adjustments in BRAN2. This leads them to conclude that the performance of BRAN3 is more dynamically consistent than BRAN2, rendering it more suitable for a range of applications, including analysis of ocean variability, extreme events, and process studies.

The key improvements in BRAN3, compared to BRAN2, include the adoption of a new data assimilation algorithm, where the matrix inversions are performed in ensemble-space instead of observation space; improved treatment of the observations; the adoption of an “adaptive nudging” approach to model initialization (Sandery et al. 2011); and the explicit updating of temperature, salinity, and velocity only – with no explicit adjustment to sea-level. Along with other less significant changes, the BRAN3 system out-performed the BRAN2 system in almost all aspects.

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AWARDS

Dr. Oke was the recipient of the 2012 IMarEST Denny Silver Gilt Medal – presented to the best paper published in the Journal of Operational Oceanography in a calendar year; for "GODAE inter-comparisons in the Tasman and Coral Seas".